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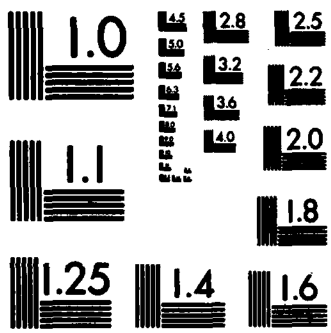

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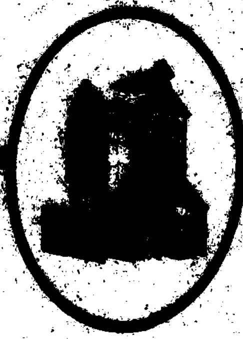

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These three volumes constitute the written contributions of speakers at the International Conference on Stiff Computation, held April 12-14, 1982, at Park City, Utah. As this collection was prepared in advance of the meeting, a few contributions were too late to be included here. The purpose of this meeting was to bring together theorists, software developers, and users on common ground to consider the state of the art - and practice - of stiff computation. Most of the papers in these proceedings will appear formally in the form of a monograph.

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PROCEEDINGS OF THE INTERNATIONAL CONFERENCE ON STIFF COMPUTATION

April 12-14, 1982
Park City, Utah

Volume I

THESE PROCEEDINGS ARE
DEDICATED TO THE MEMORY OF
PROFESSOR LEON LAPIDUS
PRINCETON UNIVERSITY

A

INTRODUCTION TO THE PROCEEDINGS

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Richard C. Aiken
Conference Chairman

A

CONTENTS

VOLUME I

Volume I consists of:

VOLUME II

APRIL 12, 1982

(In Order of Presentation)

F.C. HOPPENSTEADT (speaker),
P. ALFELD, University of Utah:

EXPLOSION MODE ANALYSIS
OF AN H_2-O_2 REACTION

W.L. MIRANKER, IBM:

AN OVERVIEW OF THE HIGHLY
OSCILLATORY INITIAL VALUE PROBLEM

R.M.M. MATTHEIJ, Katholieke Universiteit,
Netherlands:

RICCATI TYPE TRANSFORMATIONS AND
DECOUPLING OF SINGULARLY PERTURBED ODE

R.E. O'MALLEY, JR., Rensselaer Polytechnic
Institute (speaker),
R.M.M. MATTHEIJ, Katholieke Universiteit:

DECOUPLING OF BOUNDARY VALUE PROBLEMS
FOR TWO-TIME SYSTEMS

T.A. BICKART, Syracuse University:

P-STABLE AND $P(\alpha,\beta)$-STABLE
INTEGRATION/INTERPOLATION METHODS
IN THE SOLUTION OF RETARDED
DIFFERENTIAL-DIFFERENCE EQUATIONS

D.J. Nolting, USAF Academy (speaker),
D.J. Rodabaugh, Lockheed:

STIFFLY STABLE LINEAR MULTISTEP METHODS

S.O. FATUNLA, Trinity College, Dublin:

P-STABLE HYBRID SCHEMES FOR INITIAL
VALUE PROBLEMS

APRIL 13, 1982

G. DAHLQUIST, The Royal Institute of Technology:

SOME COMMENTS ON STABILITY AND ERROR ANALYSIS FOR STIFF NONLINEAR PROBLEMS

W. LINIGER, IBM:

CONTRACTIVITY OF MULTISTEP AND ONE-LEG METHODS WITH VARIABLE STEPS

J.R. CASH, Imperial College of Science and Technology:

A SURVEY OF RUNGE-KUTTA METHODS FOR THE NUMERICAL INTEGRATION OF STIFF DIFFERENTIAL SYSTEMS

W.E. SCHIESSER, Lehigh University:

SOME CHARACTERISTICS OF ODE PROBLEMS GENERATED BY THE NUMERICAL METHOD OF LINES

B.A. FINLAYSON, University of Pennsylvania:

SOLUTION OF STIFF EQUATIONS RESULTING FROM PARTIAL DIFFERENTIAL EQUATIONS

S.W. CHURCHILL, University of Pennsylvania:

STIFFNESS IN HEAT TRANSFER

J.O.L. WENDT, University of Arizona (speaker)
W.A. HAHN, Exxon Production Research Center:

INTEGRATION OF THE STIFF, BOUNDARY VALUED ODE'S FOR THE LAMINAR, OPPOSED JET DIFFUSION FLAME

J.E. DOVE, University of Toronto (speaker),
S. RAYNOR, Harvard University:

A MASTER EQUATION STUDY OF THE RATE AND MECHANISM OF VIBRATIONAL RELAXATION AND DISSOCIATION OF MOLECULAR HYDROGEN BY HELIUM (abstract)

C.A. COSTA (speaker), M.Q. DIAS, J.C. LOPES, A.E. RODRIGUES:

DYNAMICS OF FIXED BED ADSORBERS (abstract)

F.E. CELLIER, ETZ-Zurich:

STIFF COMPUTATION: WHERE TO GO?

VOLUME III

APRIL 14, 1982

C.W. GEAR, University of Illinois at Urbana-Champaign:

STIFF SOFTWARE: WHAT DO WE HAVE AND WHAT DO WE NEED?

W. H. ENRIGHT, University of Toronto:

PITFALLS IN THE COMPARISON OF NUMERICAL METHODS FOR STIFF ORDINARY DIFFERENTIAL EQUATIONS

A.C. HINDMARSH, Lawrence Livermore National Laboratory:

STIFF SYSTEM PROBLEMS AND SOLUTIONS AT LLNL

G.K. GUPTA, Monash University:

DESCRIPTION AND EVALUATION OF A STIFF ODE CODE DSTIFF

P. DEUFLHARD (speaker), G. BADER,
U. NOWAK, Universitat Heidelberg:

AN ADVANCED SIMULATION PACKAGE FOR
LARGE CHEMICAL REACTION SYSTEMS

L. EDSBERG, The Royal Insititute of
Technology:

CHEMICAL KINETICS - AN OVERVIEW FROM THE
POINT OF VIEW OF NUMERICAL ANALYSIS AND
SOFTWARE IMPLEMENTATION

J. DEVOOGHT, Universite Libre de Bruxelles:

AN OVERVIEW OF STIFFNESS PROBLEMS IN
NUCLEAR REACTOR KINETICS

S. THOMPSON (speaker),
P.G. TUTTLE, Babcock and Wilcox:

THE SOLUTION OF SEVERAL REPRESENTATIVE
STIFF PROBLEMS IN AN INDUSTRIAL ENVIRONMENT:
THE EVOLUTION OF AN O.D.E. SOLVER

P.G. BAILEY, E.P.R.I. (speaker), P.V.
GIRIJASHANKAR, D.L. HETRICK, W.N. KEEPIN and
O.A. PALUSINSKI, University of Arizona:

MULTIRATE INTEGRATION ALGORITHMS APPLIED
TO STIFF SYSTEMS IN NUCLEAR POWER PLANT
SIMULATION

S.K. DEY, NASA-Ames Research Center:

APPLICATIONS OF PERTURBED FUNCTIONAL
ITERATIONS TO NONLINEAR STIFF INITIAL
VALUE CHEMICAL KINETIC PROBLEMS

J.-T. HWANG, National Tsing Hua University,
Taiwan:

NONLINEAR SENSITIVITY ANALYSIS IN
CHEMICAL KINETICS--THE SCALED GREEN'S
FUNCTION METHOD

K.E. CHEN, Bethlehem Steel Corp. (speaker),
W.E. SCHIESSER, Lehigh University:

SOME EXPERIENCES IN THE SELECTION OF INTEGRATORS FOR LARGE-SCALE ODE PROBLEMS IN CHEMICAL ENGINEERING

STIFF REVIEW 1974-1982: I. APPLICATIONS

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April 12, 1982

INTRODUCTION

It is the responsibility of the practitioner, that is the engineer or scientist, to develop the simplest model that explains or predicts variables of interest. The implications of not enough model detail are much better appreciated than the implications of too much model detail. If the entire system model identification and parameter estimation proceed interactively with experimentation and data acquisition, the appropriate model should result.

When this does not happen, the major likely reason is: the model of the overall system is typically formed from many small sub-models and parameters are estimated from data on the submodels. Consider, for example, the kinetic model for combustion of a hydrocarbon. Hundreds of reactions may be theoretically possible to occur although the vast majority may not need to be considered in order to predict, say, the overall burning rate. However, typically the big model is formed and then data taken from experiments on many small submodels, here consisting of the individual reactions. Data may be retrievable for this single reaction or for a small sub-set of reactions, but it may not be important or desireable to do so.

The numerical penalty for too much model detail is too much computation time, either because the system is larger than needed or because the system is stiff, or both. I mean here to use this

term stiff as the Webster anonym "subborn"; thus included in this review are highly oscillatory systems, "stiff" two-point boundary value problems, discontinuities, and stiff boundary vaule problems. For a precise definition of stiffness see Shampine(1982); also the versions of Watson(1976), Robertson(1976); Scherer(1976); Lambert(1980); Seider(1980); and Gear(1980). Guderley(1975) defines stiff two-point boundary value problems.

There is another fundamental problem with the identification and estimation stage beyond the inappropriate model detail that results: the basis for the derived parameters is wrong. Pretend that you must design a process for separating two liquids by boiling them, condensing the resulting vapor and then boiling again in stages (distillation). A major parameter need for your design equations would be the relative volatilities of the components as a function of composition. This can be done in a simple bomb experiment in the laboratory followed by least-squares fitting the data to an assumed function; but in doing this you have obtained results optimal at best to your rather arbitary least squares criterion. What you really want is to minimize the uncertainty in the design of your process, and this should be expressed at the parameter estimation stage.

Let us consider now the case where we in fact do a "systems" identification and parameter estimation on a detailed dynamic

model. We then face the inverse problem of stiff numerical solution - stiff parameter estimation. This not only can present huge experimental requirements but the need also for special mathematical and numerical considerations (Aiken, 1982; Aiken and Venkateschwaran, 1982).

It is implicitly assumed in most all the papers in this review that a stiff model is desirable from a predictive standpoint and that the parameters are appropriate and correct for the model. If this is not true, then model simplification may be in order. The steady-state approximation applied (properly) a posteriori, or after the model and data, is a mathematical approximation(Aiken and Lapidus, 1974; Aiken and Lapidus, 1975); but the same reasoning applied a prori is just a modelling decision. So this approximation can be a very reasonable, and powerful, strategic approach before attacking with the stiff artillery.

There is considerable overlap amonst the stiff application areas listed below. An effort is made in each area to explain why the models are stiff and what some of the researchers did to overcome the numerical simulation difficulties. Industrial laboratories are explicitly noted.

ATMOSPHERIC

Description of atmospheric phenomena involves transport with chemical reaction; stiffness can occur because the time scales of the reactions are much smaller than times for transportation over distances of interest. The transport equations themselves can be stiff because these distances can be very long indeed; and the chemical kinetic rate equations are usually large and usually stiff. Pollutant formation models naturally are stiff because highly reactive free radical transients are included in the model as they are intimately related to formation of trace quantities of polutants.

Several very effective packages have been developed at Lawrence Livermore National Laboratory for the solution of differential equations modelling atmospheric phenomena (Byrne, 1981; Hindmarsh, 1982). EPISODE was written for stiff chemical kinetics including minor species in the upper atmosphere. It has solved successfully such problems with diurnally varying reaction rates. EPISODE has been modified (EPISODEB) for problems that also include transport. The modification is to recognize the banded structure of the large Jacobian resulting from the method of lines and thus to handle this matrix more efficiently. If finite elements or collocation-B-splines are used on the partial differential equations, the resulting form

$$A(y,t)dy/dt=f(y,t)$$

where A is of a banded form is best handled by another version of EPISODE, EPISODEIB. Systems of this type include differential-algebraic sets if A has one or more zero columns. Carmichael et al.(1980), for example, applied the Galerkin finite element method to the movement of pollutants in the atmosphere.

Brown(1980), however, used EPISODE for solution of a diurnal kinetics example and judges it too inefficient. Here some concentrations are small during the night, suddenly increase by orders of magnitude with the first coming of light, vary slowly during the day with maximum values around noon, and then drop sharply at sunset. With the cycle time well-know, Brown transforms the time coordinate to stretch it during the times of rapid change; in the transformed time the step size is more constant.

Miller et al.(1978) present a one-dimensional model of atmospheric fluorocarbon-ozone photochemistry with transport. Chang et al.(1974) solve over 14,000 ordinary differential equations to describe the effect of the SST on the ozone layer.

Bottenheim and Strausz(1980) modeled gas-phase chemistry in clean air as a prelude to including polutants. Gelinas and Skewes-Cox(1977) explore tropospheric photochemical mechanisms. Baldwin et al.(1977) study rate parameter estimates in a photochemical smog kinetics model. Atkinson et al.(1980) did a modeling study fo the gas -phase NOX-air photoxidation of toluene

and the cresols. Pitts and Finlayson(1975) propose various mechanisms of photochemical air pollution. Preussner and Brand(1981) apply a semi-implicit Euler method to photochemical smog kinetics. Kuhlman et al.(1978) study the effect of CO on sulfate aersol formation. Wallace et al.(1980) model photochemical ozone and NO formation. Watkins(1981) solves an ionospheric model with several unknown initial conditions; these are chosen so to avoid the initial steep transient(see also Aiken, 1974, for problem approximations like this). Isaacson(1981) predicts extremely high wind speeds at ground level on the downstream side of a mountain range.

Difficulties with the use of steady-state approximation on the stiff reaction rate equations has been pointed-out by Farrow and Edelson(1974). Reasons could include: the necessity of including in the model radicals which very directly effect the trace variables of interest; the re-occuring nature of the stiffness on a daily basis; the typically large size of the equation set makes choice of stiff variables more difficult. Dickinson and Gelinas(1976) performed sensitivity analysis on these types of equation to better understand what reactions are important in their example. Farrow and Graedel(1977) found the steady-state approximations applied to some species but not to others that they would have expected to work; some species rates can have this approximation hold at various diurnal times.

BIOLOGICAL

Most chemical reactions occuring in living species involve a catalyst that helps with proper orientation of the big floppy biological molecules. The catalyst is called an enzyme. These reactions are stiff for one of two reasons: 1. There is typically a large scale difference between the concentration of the reactant, called the substrate, and the enzyme, or 2. There is a large difference in the rate constants. Aiken(1982) explores the validity and the implications of the so-called Michaelis-Menten(M-M) approximation to relieve the stiffness and presents a number of other approximations. These could be more valid depending upon the relative magnitudes of the rate constants.

It has been historically rather rare to find enzyme models where the M-M approximation has not been used. The reason for this seems to be primarily an experimental limitation: the enzyme-substrate complex, typically the stiff intermediate variable, is like the enzyme itself present in very small quantities and may not differ greatly from measureable characteristics of the enzyme or the substrate. It was measured spectroscopically at about mid-twentieth century and allowed the first complete model of enzyme kinetics with all parameters specified. There seems to be a growing interest in obtaining this (stiff) model detail today (Hiromi, 1982; Kondo, et al., 1980). Kinderlehrer and Ainsworth(1976) have written a program to

predict detailed enzyme mechanisms with all intermediates.

In addition to enzyme kinetics stiffness appears in pharmocological compartment models of drug response. Gehring and Blau(1977), of Dow Chemical, have modeled dose response to suspected carcinogens and noted the initial large transients. Bloch et al.(1980) found the processes of reversible binding of drug to protein occurs rapidly on the time scale of the solution to the drug disposition in the body. Jackson(1980) used a version of GEAR for the kinetic simulation of anticancer drug interactions. Perelson and DeLisi(1980) encountered stiffness with receptor clustering on a cell surface. Perelson(1979) found that an antigen will come on and off the surface of a cell many times before cross-linking occurs. Karba et al.(1980) use hybrid computer simulation to overcome stiffness in drug pharmoco kinetics.

Loomis et al.(1979) ,in modelling crop physiology, found that while he was interested in crop growth over a period of many days, he had to use a time scale of hours to include diurnal events or a scale of minutes or seconds if cellular process were to be included. Chu and Berman(1974) developed a program using an exponential method for modelling and simulation of complex biological systems. Gottwald and Wanner(1982) compare various methods for stiff differential equations occuring in biology. Hunding(1980) came across stiffness and "chemical histeresis" in

simulating a biological cell or early blastula.

COMBUSTION

This is a special area of reaction with transport and of chemical kinetics. Stiffness can come from the time scale differences between reaction and transport or from the stiff kinetic system or from both.

Combustion kinetics could be defined as simply describing oxidative-type reactions, but the primary reactions of interest are initiated by combination of oxygen with hydrocarbons. From this class the most important reactions are the chain branching type or autocatalytic reactions that proceed ever faster as fuel is consumed - explosions. Most combustion applications involve explosive reactions confined in space; the spacial location of most intense reactivity is termed the flame heart. Aiken(1982) explores the definition of the term "explosion" and develops criteria for the degree of explosive activity for the oxygen-hydrogen problem.

Stiffness in explosive reactions is different from that in most other kinetic systems in that fast transients do not occur only for initial times but usually appear later in the transient. Thus codes that are taking giant time integation steps can jump over the explosive zone where most of the action is. Another difference is that the stiff variables change during the transient. Typically at least three major time scales are

important in these systems: initiation, "explosion" and termination. For all these reasons stiffness in combustion kinetics can be particularly severe; only recently has the steady-state approximation been successfully and automatically applied to these reactions (Aiken, 1982). Hoppensteadt et al.(1981) presents a projection method that focuses on the positive eigenvalue during the explosion. Pratt(1979) has investigated special methods that make use of the special structure of the kinetic equations. See also White and Seider(1981).

Addition of the spacial variable further complicates the potential numerical problems. The flow in which combustion occurs is usually turbulent with intermittent changes on time scales different from the kinetic time scales. Stochastic methods are promising for overcoming this stiffness (Chorin, 1980). Kansa (1981) ,of the Lawrence Livermore National Laboratory, has combined some aspects of block implicit PDE schemes with stiff ODE solvers for this problem; this was partially motivated by the experience that block implicit methods, although unconditionally stable for linear equations, were found to have inadequate stability properties for the severe nonlinear Arrhenius temperature dependence of the reaction rate.

Operator splitting techniques are often used for the

numerical solution of multicomponent gas mixtures undergoing rapid reaction. They offer better storage economy than fully implicit schemes and better stability properties than explicit schemes; their low order accuracy is appropriate, and they allow flexibility and modularity in the overall numerical attack. Karasalo and Kurylo (1981), also of Lawrence Livermore, discuss in this context ways to reduce overall computation time by improving the efficiency of the stiff kinetics step at each grid point where by far the most time is spent. They employ a stiff ODE package (like GEAR) but with the following modifications: First, they avoid repeated evaluations of the Jacobian at each mesh point by storing selected historical values from adjacent mesh points. Second, they allow step sizes and order to vary more frequently since this is not the expensive feature. Thirdly, they artifically impose that concentrations remain non-negative during prediction and corrector iterations. This last point is an important one as it has been found that small negative concentrations that can result from rounding or truncation causes stability probems that require a local error bound smaller than that otherwise sufficient for a given global accuracy request.

Otey(1978), of Sandia, formulated a test problem with combustive reaction and diffusion to make comparisons among solutions by the method of lines, linearized block tridiagonal

procedures, and other techniques. He found the block diagonal implicit procedure was by far the best in all variants of the test problem, including ones for which the system was quite stiff through stiffness in the kinetic equations. Wendt et al.(1979) and Wendt(1982) present methods for solving stiff boundary-value problems with combustion and diffusion in a pore. The reaction occurs on the surface of the pore. A variable grid mesh is used so as to be finer at the pore mouth where concentrations change fastest. Sundaresan and Amundson(1980) also report the very stiff nature of this problem.

Oran and Boris(1981) present a comprehensive exaimination of modelling and simulation of combustive flow problems. They also mention that kinetic ODE stiffness within a spacial model cannot be handled adequately for realistic models because the usual matrix inversions would be too expensive for a large number of chemical species and many grid points; storage is also an obvious big problem. These authors review the very complex nature of modelling and simulating turbulence for reactive environments.

Sandusky et al.(1979) advocate finite element techniques for combustive transport. Westbrock(1978) offers an improvement in th operator splitting method. George and Harris(1977) lament stiffness from a model of in situ oil shale retorting. See also Scaccia and Kennedy(1974) , McDonald(1979), Choi and Churchill(1979), and Lowe et al.(1977).

CONTROL

Many engineering control systems can be modelled by the form:

$$dx/dt = Ax + Bz$$
$$e\, dz/dt = Cz + Bu$$

where the first equation represents a large linear multi-variable plant, and the second equation represents a multivariable actuator. e is a small parameter that indicates a fast contoller response in comparison to plant variable time scale. The controller might be electrical and the plant mechanical or involving fluid transport.In general e cannot be neglected (set equal to zero) since the presence of the controller dynamics can govern the inherent stability of the plant-controller complex; see Porter(1976), however, for some conditions for which this simplification is permissible. Shimizu et al.(1980) describes some stiff nonlinear control problems.

This singularly perturbed simple linear form has been exploited by Khalil and Kokotovic(1980) in the design of decentralized feedback controlers. Anderson(1980) offers a time-varying transformation to separate the fast from the slow modes. Dontchev(1974) explores by sensitivity analysis optimal control systems with changes in order. Womble(1976) looks at some further approximations to Ricatti equations having fast and slow modes.

Any differential equation can be considered stiff if a

solution is required in a short enough computing time. Real time aerospace control applications can have this feature. Bulirsch and Branca(1974) mention for an optimal deceleration maneuver an Apollo-type vechicle would need information in about one second and would allow up to 1% error.Gear (1977) discusses the conflict between real-time and software; he mentions that real-time implies that implicit methods cannot be used in the usual sense and presents some of the semi-implicit methods. See Hiestand and George(1976) for other stiff aerospace applications.

Ojika et al. (1979) give a "time decompostion" algorithm for a stiff two point boundary value problem applied to nonlinear optimal control problems.

DISPERSED PHASES

Consider a liquid or solid phase dispersed as droplets or particles in another gas, liquid or solid phase. If the size distribution of the dispersed phase is broad, stiffness can result from models that include heat or mass transfer, particularly complex when reaction is also occuring in the dispersed phase. This is because it is much easier to transport mass and heat to smaller sizes, roughly proportional to the reciprocal of the effective diameter. For example, Kayihan(1980) describes a model and solution for coal devolatilization in which heat is transfered preferentially to the smaller particles that

therefore devolatize relatively rapidly and cause severe numerical simulation problems. As usual, a modelling choice must be made as how small a size to include. The size distribution functions typically have a skewed maximum with long tails - particularly in the direction of the smaller sizes. The modeller must often determine a cut-off point for small particles; smaller than that would cause numerical problems but ideally not contribute significantly to the solution variables of interest.

Wall and Anlansson(1980) use a version of the GEAR package to solve a model of stepwise micelle association. Lahey et al.(1980) also use this package for modelling bubbles flowing through a nozzle.

See also the sections in this review on heat transfer and reactors. Bubble columns and spray reactors can exhibit this type of stiffness as can processing crushed shale or coal. This problem can be particularly severe in the case of in situ solids processing for which the particle sizing from underground explosions, for example, is widely varying.

ELECTRONICS

The time domain analysis of electronic circuits requires the solution of nonlinear algebraic-differential equations. Implicit integration methods and sparse matrix techniques made possible analysis of circuits containing hundreds of active devices.

Advances in large-scale integrated circuits have indicated potential for analysis of thousands of active elements. Hybrid method simulation is an interesting concept that applies different methods to sections of the circuit that require different accuracy, but effects of interaction among the subsystems can be difficult to assess a priori. The concept of "latency", rather like a temporary steady state approximation, has also received attention in this area. The relationship between latency and the numerical method has been explored in Rabbat et al.(1979), of IBM Data Systems Division. See also Tadeusiewicz(1981).

Power system dynamic response involves the solution of large differential-algebraic equations. The differential equations model the dynamics of the machines and their control systems while the algebraic equations model the network steady-state relationships. Gross and Bergen(1977) pursue this combination by partitioning the set into a non-stiff part and a stiff part with a sparse Jacobian matrix.

Resonant circuits, time variant and time invariant, have been studied by Ruehli et al.(1980), of IBM T.J. Watson Research Center. "A-contractive arc" methods were shown to perform well for both types of circuits. Oscillatory nonlinear circuits with a finite number of continuous derivatives has been the subject of

work by Hajj and Skelboe(1979). Zein(1980), of IBM Data Systems Division, discusses the use of "sensitivity circuits" for the transient analysis of periodic circuit behavior.

A range of integration algorthms have been tested on some model problems of large ODE sets for power system dynamics by Humpage et al.(1974). Methods for fast contingency analysis at a power systems control center are advanced by Chamorro et al.(1981).

Alvarado(1979) reports some results on stiff transient stability analysis of circuits. Weaver et al.(1977) give a stiff model for radiation-induced bulk electrical conductivity in insulators. Covello and White(1977), of the U.S. Air Force Weapons Laboratory, discuss stiffness when investigating radiation response characteristics of networks.Charge transfer in a nonlinear stiff model of charge-coupled devices has been simulated by McKenna and Schryer(1975), from Bell Labs. Warner and Wilson(1980), also working at Bell Labs, use some analytic transformations to help lessen the stiffness from their equations related to the fabrication of narrow-channel MOS transistors. Gambart-Ducros and Maral(1980) concern themselves with the stiff differential equations that arise from some computer aided design techniques; see also Dietze and Reibiger(1978). Von Pragenau (1981) reports his own method for greatly reducing the computation time of stiff digitial filters. Stiff nonlinear

switching circuits has been attacked by Boness(1979) and specifically switching serges byTripathy and Rao(1978).

See the section in this review on control systems for some further stiff applications involving electronics.

FLUIDS

Stiffness occurs in spacial coordinates within homogeneous fluids with sharp changes in physical properties or from abrupt obstructions in the flow path. Compressable flow with compression and rarefaction (shock) waves, reflection, flow reversal and choked flow all can lead to numerical problems.

The method of characteristics is "characteristically" used on problems of inviscid flow because it naturally handles discontinuous derivatives as it follows waves but cannot be used on viscous shock layer equations. Srivastava et al.(1979) present a finite differencing scheme for viscous flow past blunted cones, where derivative discontinuities are encountered at the sphere-cone juncture point. To avoid large truncation errors associated with these points, differencing across the discontinuity is carefully avoided. The method of characteristics can become too expensive on inviscid flow problems to follow long term transients involving shock waves; Carver(1980) gives a spacial discretization which utilizes the directional aspects of the method of characteristics.

Blottner(1980), from Sandia Laboratory, used a variable grid approach to solve turbulent boundary-layer flows that involve jumps in viscosity and density. Blottner has used both coordinate stretching with uniform grid in the stretched coordinate as well as discontinuous grid spacing that is effective for discontinous changes in variables. MacCormack and Paullay(1974) ,of NASA Ames, provide a study on the effect of the mesh spacing on inviscid supersonic shock flows. Stewart(1979), of the Atomic Energy Laboratory in France, examines a model-oriented numerical method for solving flow with sharp changes in phase as occurs in cooling water superheated locally. Other variable mesh approaches are shown by the Russian group of Yanenko(1979) for boundary layer shear flows.

The PDEs that model unsteady flow in one, two or three dimensions can yield stiff ODEs when spacially discretized - the method of lines. This will be the case where there are many spacial grid points compared to the time steps that one would like to use. A large number of spacical mesh points can result from tight spacial coupling or simply from "long" distances to be covered. The method of lines can be attractive because of its programming simplicity but is not as efficient as finite differencing for problems without tight spacial coupling (Kurtz et al., 1978).

Madala and Piacsek(1977) ,of the U.S. Naval Laboratory, have

studied numerically the responce of oceans to weather changes. They avoid small time steps associated with fast moving surface gravity waves by dividing the flow into baroclinic and barotropic vertically averaged modes; the baroclinic waves are treated explicitly and the barotropic waves implicitly (still computation times reach over 60 hours on a large computer).

See also Coleman et al.(1977) for averaging methods applied to stiff circulatory flow and Gersting(1980) for the Orr-Somerfield flow approached as an initial value problem. Issacson(1981) looks at the mountain wind problem and suggests a filtering scheme and a hybrid method for handling shocks in the atmosphere.

Refer to sections in this review on combustion, reactors, atmospheric problems and general reaction - diffusion for flow problems with reaction coupled to transport.

HEAT

Stiffness in heat transfer originates in one of two ways: sharp changes in temperature environment or large differences in the rates which components of the system can transfer heat. The first problem could be a boundary-value problem with the sharp changes represented in the boundary conditions. A realistic model for these boundary conditions is a tough problem in itself since discontinuities would not exist in nature; step changes in

temperature can result in infinite heat fluxes, certainly not observed. The other class of stiff heat transfer problems arise from differences in heat capacities or by size differnces among the components. For this category see also the section on dispersed phase transport where, for example, heating of coal particles for pyrolysis is discussed.

Krishnan and Sastri(1978) solved the thermal entry length problem for high Prandtl numbers, that is, with large differences in heat flow, by convective versus conductive means. The Russian group of Mazhukin et al.(1980) dealt with stiffness that occured through large spacial temperature differences created through laser irradiation of targets and interaction with the resulting plasma above the surface. This type of stiff heat problem commonly comes from non-isothermal chemical kinetics coupled in a model with transport; refer to the sections in this review on combustion and on reactors.

Mention also should be made of the stiff set of ODEs that result from discretization of the PDEs that describe unsteady heat transport. See, for example Bushard(1976) ,who solves the heat conduction equation with the method of lines. Wood(1977) discusses the solution of the stiff equations that result from a finite element discretization of the heat conduction equation.

Distillation is a chemical engineering heat transport

process that can result in stiff numerical models because of differences in the liquid hold-up in the big boiler at the bottom of the column compared to the much smaller hold-up on the plates. If dynamics of the vapor traffic is included together with that of the liquid, stiffness occurs throught the great difference in heat capacities between the liquid and the gas. Tyreus et al.(1975) examined stiffness in a specific model of a distillation tower and found it became more severe the more difficult the separation (from high purity requirements or from the components to be separated being similar in their volatilities). An adaptive semi-implicit Runge-Kutta algorithm was used by Prokopakis and Seider(1980) in a model in which the rapidly changing liquid flow rates were decoupled in a sense from the relatively slowly changing mole fractions. See also Seider(1982). Ozoe et al. tackle a stiff thermoacoustic convection problem.

This type of stiffness from heat capacity differences very commonly occurs in reactors which contain two or more phases. For example, a reactor tube containing a solid particle packing that is processing a gas will experience stiffness if the dynamics of the temperature change in the solid and gaseous phases are included in the model.

See also Churchill(1982) for a review of stiff heat transport problems.

CHEMICAL KINETICS

This is by far the largest stiff application area. Stiffness is caused in the vast majority of cases simply by a large difference among the reaction rate constants. The larger the system or the more detailed the model, the more likely that stiffness will occur. If the elementary reactions are known, the "law" of mass action dictates the form of the rate expressions: either linear in a concentration variable or quadratic.

Several investigators have made use of this special simple structure of mass action kinetics. Edsberg(1974); Edsberg(1976); and Edsberg(1982) make the problem set-up, Jacobian evaluation simplified for the user and efficiently handles the Jacobian, but Dahlquist et al.(1980) feel more can be done to make use of structure as well as the users' knowledge of the stiffness. This knowledge often consists of: a partitioning of variables into "stiff variables" and "non-stiff variables."; a fast transient that occurs initially only; inherent tight stability of the stiff variables whose concentrations must not be negative. Karasalo and Kurylo(1980) point-out an advantage in keeping these concentrations artifically non-negative when using a version of GEAR. Robertson(1975, 1976) also suggests some structure-related handling of the Jacobian for faster convergence.

Packages exist specifically for the mass action kinetics form. Uhlen(1979) describes KINRATE and KINBOX. Edelson(1976), of Bell Laboratory, presents a simulation language and compiler for mass action kinetics; he uses a version of GEAR in forming a

package called BELLCHEM. Rider(1977) offers CAKE, user friendly version of GEAR that makes use of the typical sparse structure of large mass-action kinetic equations. Deuflhard et al.(1981)and Bader et al.(1982) describe LARKIN to handle large systems of kinetic equations. Gottwald(1981) gives us KISS for coupled chemical reactions. Stabler and Chesick(1978) have also written a program for reaction rate equations using a version of GEAR.David(1977) describes a FORMAC program for direct integration using formula manipulation and a Taylor-made numerical method; Kennedy and Moore(1977) also recognized the virture in using a Taylor-series expansion as the basis for a numerical method with such simple functions.

Enright and Hull(1976) compare numerical methods for stiff kinetic problems and found that the backward differentiation methods were superior to most other methods, including an implicit Runga-Kutta technique; pitfalls in generalizing such conclusions are explained by Enright(1982).

The steady-state approximation has been extensively used to eliminate stiffness in chemical kinetic systems(Aiken and Lapidus, 1975). Noyes(1978) discusses the importance of including reversible reaction when the approximation is made.

Sensitivity analysis is becoming an effective means of determining appropriate model detail. Koda et al.(1979) studied

automatic sensitivity analysis of kinetic mechanisms and developed FAST (Fourier amplitude sensitivity test). Dougherty and Rabitz(1980) look at the sensitivity of hydrogen combustion. Rabitz gives an overview of this area applied to chemical kinetics. Hwang(1982) has a means for nonlinear sensitivity analysis in chemical kinetics. See also Kuchel(1980), Sundaresan and Amundson(1980), Dougherty et al.(1979), Dove and Raynor(1979), Dickinson and Gelinas(1976), and Lowe et al.(1977).

A specific kinetic application area not covered within any of the other sections of this review is pyrolysis. Hautman et al.(1981) mention that at low conversions the primary reactions govern the dynamics, but at higher conversion the secondary reactions do. Layokun and Slater(1979) model a free radical mechanism of propane pyrolysis and solve it with a semi-implicit trapezoidal rule. A number of thermal cracking models were solved in detail by Sundaram and Froment(1978). Liquid phase pyrolysis of 1,2 diphenylethane was studied by Miller and Stein(1981).

An overview on the computational techniques for the study of reaction processes is avaiable from Edelson(1981). A stiff model for chemistry in interstellar clouds is advanced by Prasad and Huntress(1980). Ross(1977) mentions the problem of loss of detailed balance when applying the steady-state approximation and does this instead by a Markov matrix method. Rosenbaum classifies certain numerical methods as "conservative" (satisfying the

detailed balance) or not. Ong and Mason(1976) discuss a different type of stiffness in kinetic systems than the type we have been implicitly focusing on: one in which the right hand side is the difference of two large terms; they convert the initial-value problem into a two point boundary-value problem for the case that the right-hand side passes through zero. See also the entire volume 81, number 25 pp 2309-2559 of the Journal of Physical Chemistry(1977).

LASERS

Lasing results from creating a highly excited vibrational state in a group of molecules("pumping" to an inverted energy state). Then a remarkable fact of nature dictates that whatever the "relaxations" back to lower energy states that begin, the resulting photons will stimulate other of the still excited energy states to relax in the same way, creating an autocatalytic effect - and coherent radiation. These relaxations are very fast and one source of stiffness in the modelling of lasers. Shampine and Gear(1979) point out that the fast pump-emission, pump-emission cycle of the various energy levels is a re-occuring stiffness that cannot be dealt with effectively with typically available automatic stiff packages. This is because fast transients occur through-out the solution so accuracy in handling these transients can be continually important. Cukier and

Levine(1978) mention use of a steady-state approximation during the lasing action, but details on this apparently ad hoc approach were not given. There is an initial fast transient from the onset of pumping (Milonni, 1977), that is at t=0.

Cukier and Levine also examine the sensitivity of the full solution for a model of an HF chemical laser and find only a few of the rate constants are responsible for the computed gain. A more detailed model of an HF laser is given by Ben-Shaul and Feliks(1979)and by Kerber et al.(1977). It should also be mentioned here that the rate consants, particularly the fastest ones are only known very approximately, errors of several orders of magnitude are not uncommon.

High energy lasers usually use a gas as the lasing medium for best efficiency and as a flowing medium to remove heat. The addition of flow can require the laser model to include hydrodynamics coupled to the chemistry. The time scales of transport versus reaction are much different here (see also sections on reactors and combustion). Inclusion of hydrodynamics, translational and rotational energy interactions, wall effects and the like are necessary to actually predict the perforamnce of the laser - to compute how much power output can be extracted and its nature. Additional sources of stiffness can result from the variety of time scales amonst the three very different types of

energy transitions for a molecule: vibrational, rotational, transulational (see the section in this review on molecular dynamics). A molecule in a particular energy state of the many potential combinations is considered a distinct species, so that a large number of highly interactive species can result from only a few different molecules.

A meeting conviened at the U.S.Air Force Army Weapons Laboratory brought in stiff experts Shampine, Gear, Liniger, Hindmarsh, and Byrne to lecture on stiffness and hear several talks by laser modelers. Some of these have been referenced above, others are: Franklin(1977) who spoke on modelling general kinetic processes in lasers; Lundstrom(1977), of the Naval Weapons Laboratory, on modelling the CO laser; Holmes(1977) on CO2/N2 vibrational kinetic equations; Hines on CW CO2 electric discharge modelling; and Young and Boris(1977), of the Naval Research Laboratory, on general numerical techniques for chemical kinetics with reactive flow.

Plasma chemistry has been studied as it relates to laser discharge and target interactions. The chemical reactions can include neutral molecule-neutral molecule collisions as well as electron-ion, electron-molecule, and molecule-ion collisions. Roberts(1979) presents his program PLASKEM for this problem. Pert(1978) calculates ionization in rapidly changing plasmas in a model that includes hydrodynamics but integrates these two

regimes separately in a steady-state type of approximation. The Russian team of Mazhukin et al.(1980), in a numerical investigation of laser breakdown of a dense gas, regect a version of GEAR and the method of lines for that of the Russian Samarskii(1971); his method also is a type of steady-state approximate decoupling of kinetics from transport. Christiansen and Winsor(1980) study a numerical model for laser targets, essential to the feasibility investigation of laser fusion.

Refer to Lawton et al.(1979) for numerical work on the high-pressure infrared xenon laser; Greene and Brau(1978) for KrF and ArF lasers; Barker(1980) for infrared multiphoton decomposition; Pirkle et al.(1974) for pulsed DF-CO2 transfer lasers; and to Bui(1979), Bui(1980), and Bui(1981) for model design and analysis of a new type of blast-wave induced laser.

MECHANICS

The term "stiffness" is commonly used in structural mechanics in a much different sense than the present context. The "stiffness" matrix results from a linear model

$$f=Ky$$

where f is force and y is displacement. The denser K, the "stiffer" the problem (finite elements used) in the physical sense that there are more interactions among the components. This would imply typically a more stable system, but a stiff system in

this sense is not necessarily associated with fast transients. Large second-order systems of the form

$$My'' + Cy' + Ky = f(t)$$
$$y(0),\ y'(0),\ \text{given}$$

occur frequently in the transient analysis of dynamic structures (Enright, 1980). M, C, and K are the mass, damping, and stiffness matrices, respectively. In the case of large deflections, the problem becomes nonlinear through K depending on y. Here the forcing function f(t) can make accuracy an important consideration for any component of y, including the stiff ones, at any time in the transient; the numerical stability of all components is essential. This special type of stiffness results in computational costs very dependent on requested accuracy; once a step-size has been selected it should remain relatively constant throughout the solution, there being no boundary layers. Thus fixed step-size low-order multistep methods have been commonly used, although Enright(1980) has pointed out the advantages of second-order variable step-size approaches. Jensen(1976,1974) of the Palo Alto Structural Mechanics Laboratory examines stiffly stable third-order methods for this same problem. See also Wright(1979), Von Pragenau(1981), and Addison(1980) for the linear case and Park(1975) for the nonlinear case. This last work is particularly interesting as it demonstrates methods unconditionally stable for linear problems

are not so for the nonlinear case.

Jain and Jain(1981) develop hybrid P-stable methods that improve efficiency for solving periodic problems in celestial mechanics. De Silva and Grant(1978) of NASA Ames describe research into the development of automatic structrual synthesis methods for turbine disk and blade assemblies. Second variation methods resulted in systems of stiff inhomogeneous matrix Riccatti equations.

MOLECULAR DYNAMICS

Mathematical models of atomic and molecular dynamic interaction have successfully predicted macroscopic physical properties of fluids. Only a very small quantity of the fluid can be modeled,to limit the variables to hundreds or thousands of particles. Each particle can theoretically exert a force on all the other particles, but the simplification is made that beyond some cut-off distance the force is too small to consider in the model. This causes a discontinuity in the interaction potential that is a source of error in many molecular dynamic simulations.

The strength of the interaction is a very strong function of distance. Nearest neighbors are thus lead by a rapidly varying primary force, while particles farther apart change more slowly with time. This natural partitioning by distance of the stiff from non-stiff variables has been used by Streett et al.(1978)

with a second-order Taylor series method and extrapolation to decrease computation time. Their application was to 108 methane molecules with five sites of interaction per molecule or 540 potential interactions. Adequate accuracy was established arbitrarily on the basis of satisfaction of conservation of energy to within 0.05 per cent per 1000 time steps.

The mathematical model allows "computer experiments" to be performed that could not be done in the laboratory, or would be expensive to do. Broughton and Abraham(1980) illustrate this in their study of crystal-melt interfaces. They use a variety of GEAR.

Heinzinger et al.(1978) investigated simulations of liquids with ionic interactions and found higher order integration schemes were necessary for the faster rotational motion compared to the translational motion. Rossky and Karplus(1979) studied solvation, Karplus et al.(1980) studied internal dynamics of proteins, Rossky et al.(1979) further explored solvent-solute interactions all using a version of GEAR with typical time steps on the order of E-16 seconds. In this last study, the limitation of step size was attributed to "rapid liberational motion of the water molecules and the correspondingly rapid change in the interaction energy."

Dove and Raynor(1982), Dove and Teitelbaum(1979), and Dove and Raynor(1979) offer an interesting approach to study of

vibrational relaxation in hydrogen; the relaxation was treated as a chemical kinetics problem, with each vibrational-rotational level being considered a distinct species. Reference also Gerlich et a.(1980), Haile and Graben(1980), and Powles et al.(1979) for other stiff molecular dynamic simulations.

Microscopic simulations of reacting systems has evolved separately from molecular or atomic dynamics without reaction. This area has, in addition to the time consuming potential surface evaluations, multiple times scales from mechanical versus the chemical: while some modest time frame may be enough to model motion, a reactive interaction is typically rare on that time scale - and fast. See Turner(1978) for a review of reactive molecular dynamics and consideration of how the interplay of the physical and chemical on the molecular level can influence macroscopic physical properties.

NUCLEAR

Safety considerations in this field encourage detailed dynamic models for worst-case numerical experiments, training, design, and control. Thus stiffness can be identified at the atomic stage, mechanical fuel-handling stage, spent-fuel disposal stage, or the overall process stage.

The radiolytic decompostion of water is important to both moderator and coolant chemistry in nuclear reactors, and is stiff

because of disparity of rate constants. Carver and Boyd(1979) and Boyd et al.(1980) present a model and solve it by their own stiff sparse integration method for mass action kinetics called MACKSIM. An example of stiff nuclear reactions are given in Ward and Fowler(1980), handled by a GEAR program.

Lawrence and Dorning(1977) use smoothing and extrapolation techniques on equations stiff because they include the greatly differing time constants associated with prompt and delayed neutrons in subcritical and delayed supercritical transients in a fast reactor. The so-called "prompt jump" approximation is the same as the commonly used steady-state approximation; Blenski et al.(1978) give higher order singular perturbations for this application. Thermal reactor transients are moderately stiff and prompt supercritical reactivities non-stiff.

Devooght(1980) has developed a more general steady-state method for nuclear reactor space-time kinetics as used for description of power transients in fast and thermal reactors. He gives a review of stiffness in these models in Devooght(1982).

Rapid ejection of a control rod from the center of a thermal reactor is solved by Carver and Baudouin(1976) using a version of GEAR with their own sparse matrix solver. They also solve a stiff test model of a control rod withdrawn in a direction parallel to a reactor channel. The transient is a long 200 seconds.

Electronic Associates, Inc., of West Long Branch, N.J., are

leaders in analog computer simulation of process control centers in nuclear power plants for training purposes. The real-time critical nature of this problem and the curse of dimensionality for digitial simulation explain the attractiveness of the analog approach here.

Digital nuclear process simulation has been advanced by the Electric Power Research Institute (Bailey, 1982). Patterson and Rozsa(1980) , of Lawrence Livermore Laboratory, describe a nuclear process simulator called DYNSYL, also useable for more general chemical processes. Chambers(1978) documents use of his AGR (Advanced Gas-cooled Reactor) digitial simulator for real-time solution. Thompson and Tuttle(1982) present recent software developed at Babcock and Wilcox with an interesting explanation of its historical development in this industrial environment.Halin(1976) discusses performance of conventional stiff methods on nuclear problems with discontinuities.

Borgonovi et. al(1980) investigate solution of stiff models for predicting plutonium inventory on a continuous basis. Carver(1981) discusses numerical aspects of thermal-hydraulics. Gaffney(1982), of Union Carbide Nuclear Division, surveys methods for solution of stiff oscillatory problems as arise from magnetohydrodynamic equations.

PROCESS INDUSTRIES

Refer to the reviews of Seider(1982) and Chen and Schiesser(1982). Also to Hylton(1982) for experience with CSMP. Barney and Johnson(1975) explain the incorporation of a GEAR version ordinary differential equation solver into modular simulation framework of DYNSYS;the latest version of this package, developed at Lawrence Livermore, DYNSYL is described in Patterson and Rozsa(1978). Nilsen and Karplus(1974) give a review of continuous-system simulation languages. Ockendon (1980) give a survey of dynamic simulation of Oxford industry problems.

REACTORS

Naturally a reactor model will be stiff if its kinetic equations are stiff or if there is a difference in the characteristic transport time from the reaction time, but we are concerned here with other types of stiffness originating from the nature of the reactor model. A reactor is a vessel through which reactant continuously flows in and product out; there may be multiphase flow or the reactor can contain a fixed solid phase on which reaction takes place. Introduction of each new phase increases the potential for stiffness, depending on the model detail, as different phases can have much different physical, chemical, thermodynamic, and transport properties. For example, a tubular reactor containing a solid particle phase changes its temperature much more slowly than a gas phase flowing through it.

The strong exponential temperature dependence of reaction rates can cause very sharp temperature spikes as one marches down an exothermic tubular reactor. This nonlinearity is also responsible for the existence of multiple steady states. Aiken and Lapidus(1974) give an example of a non-isothermal fluidized bed that is very stiff and posseses three possible steady-states. See also Fan et al.(1979) and Michelson(1976), who solves this problem with a semi-implcit Runge-Kutta method.

Inclusion of a diffusive or dispersion term under conditions where convection very much dominates the flow description (high Peclet numbers), leads to stiff computation (see, for example, Shah and Parakos, 1975,and Serth, 1975). Smith(1980) uses a finite element approach to this problem.Discontinuous boundary conditions for tubular reactors, often under some controversy, cause stiffness.

Interphase mass transport with reaction can produce stiff boundary-value problems inherently unstable in any direction. Aiken(1982) solves a gas purification model of simultaneous transport of two gases into a liquid where each react with a third species; one of the two reactions is much faster than the other.

Karanth and Hughes(1974) used orthogonal collocation to solve a detailed model of an adiabatic packed bed reactor, including interphase transfer to the particles and intraphase

particle transfer. Cavendish and Oh(1979) solve the equations for diffusion and reaction in a bed of poisoned automotive catalysts pellets by applying first Galerkin's method, then a version of GEAR. Guertin et al.(1977) use exponential collocation on some stiff reactor models.Rodrigues and Beira(1979) and Dias et al.(1982) model and solve stiff fixed-bed adsorbers. Eigenberger and Butt(1976) explain a technique for automatic non-equdistant grid size space for finite differences on reactors with steep gradients. Edelson and Schryer(1978) compare finite difference with finite elements for one-dimensional reactive flow. Varma et al.(1976) explore a number of computational methods for tubular reactors. Ramshaw(1980) discusses the use of the steady-state approximation in reactive three dimensional flow . Cho and Joesph(1981) solve a heterogeneous model for moving-bed coal gasification reactors and remove stiffness with the steady-state approximation.Chin and Braun(1980) solve a model of reacting flow in a porous medium; George and Harris(1977) of in situ oil shale retorting - all quite stiff problems.

See also the section in this review on combustion where reactive flow in the confines of a combustor is discussed.

REFERENCES

References are listed at the end of Part III.

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STIFF REVIEW 1974-1982: II. PACKAGES

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INTRODUCTION

The user would like to obtain the solution to his ordinary differential equation set quickly (in both his time and in the computer's time) and in a convenient form, like plots or a tabulation with automatic choice selection of where or when to report data.

The vast majority of stiff users at the beginning of the 1980's use early version of Gear's package, commonly available through users' computer centers. By numbers of users, the most common problem is probably small (less than ten or twenty equations) moderately stiff and nonlinear. It only needs to be solved to accuracy of about one per cent for qualitative understanding of the dynamic relationships among the variables.

Necessary information from the user obviously includes functional relationships and initial conditions; other important but possibly expendable instructions would be accuracy requirements and integration interval (see Klinzing(1980) for a scheme to automatically figure out this interval). Much more additional information often proves to increase efficiency of the solution, but would probably not be welcome to the average user. This includes making a decision on whether or not the system is stiff; there even has not been general agreement on the parts of the experts on what stiffness is (Shampine, 1977;1982). In this review, stiffness is used in its most general sense of "stubborn"

numerical method behavior where differential equations are involved.

The user interface for ODE solvers has been discussed by Hindmarsh(1978); a standard was developed through extensive discussions with individuals from six DOE laboratories. This effort was intended to be part of a larger effort to form a standard collection of ODE solvers, called ODEPACK.

Formation of an ODE package as automatic as possible (but with options should the user wish to specify), winning approval with numerical analysts and big users, then the public is difficult and related to the problems associated with making comparisons among packages (see the section in this review on this topic). See Thompson and Tuttle(1982) for a description of the evolution of an ODE package in an industrial environment.

Education of the user to the point where the true power of an approach can be utilized is another problem area; quite often a good numerical methods course, including solution of ODEs is not in an engineers curriculum. See "Getting the Power to the People" by Hindmarsh(1980), also "What Everyone Solving Differential Equations Numerically Should Know," by Shampine (1980). Also Curtis(1980).

Future directions to go in the development of general software is discussed in Gear(1982; 1981), Cellier(1982), and Dahlquist(1980). This includes ultimate automation such as

automatic method selection for special problems like stiff and oscillatory systems differential-algebraic sets, differential-difference sets, systems with discontinuities, sparsity, and such. Better interaction of experimentation, differential equation model identification and parameter estimation with numerical solution requirements needs to be developed (see Koda et al., 1979, for an automatic sensitivity analysis program).

METHOD IMPLEMENTATION

Package construction from a method of interest is a very big task with a number of, alas, empirical decisions. Gear(1980) discusses the alchemy side of software development. See also sections in this review on detecting stiffness, start-up, on algebraic equations, and on step-size/order selection.

Jackson and Sacks-Davis(1980) present an alternate implementation of variable step-size mutistep formulas for stiff ODE. Burrage et al.(1980) discuss implementation of singly-implicit Runga-Kutta methods. Ueberhuber(1979) suggests an implementation of defect correct methods for stiff ODE. Sacks-Davis(1980) implements fixed SD formulas with fixed-leading coefficients for stiff ODE. Hindmarsh(1979) treats software design for ODEs from PDEs.

START-UP

Gear(1980) discusses method and initial step-size selection in multistep ODE solvers. Early automatic codes like Gear's original DIFSUB required the user specify the method(stiff or non-stiff; analytic or numerically-determined Jacobian) and the initial step-size.Usually a user does not know to the appropriate order of magnitude what size the first step should be and may not know either the best method to use. The easier question of what method is the more important, but a badly guessed initial step can waste a significant amount of time or cause one to miss some interesting behaviour. Gear(1980) examines an approach that uses the initial local eigenvalues to make the (non-stiff) method selection, and high accuracy estimates at nearby points, to select a good initial step sequence and allow a high order to be used from the beginning (where it can be particularly valuable for stiff equations and problems with inital zeros).

Shampine(1978) studies the effect finite word length limits on the minimum step size has on solutions containing zeros, discontinuities, and stiff transients. He finds only in this third category should there be in practice limitations; suggestions for algorithmic ways out are given. Thus beginning with extremely small steps can be feasible as long as protective measures are present to avoid over zealous increases from there skipping interesting phenomena. Hindmarsh(1977) gives reasons why

an ODE solver may take steps smaller than the machine precision of representing the independent variable.

Gear(1980) presents Runge-Kutta like formulas which enable a high-order multi-step method to be used from the start. Only one Runge-Kutta step is needed to do this and efficency can be nicely increased automatically. The Runge-Kutta method can be viewed as an exptrapolation technique.

STEP-SIZE/ORDER CONTROL

This idea enabled Gear's backward difference method to take a "step jump" in advancing automatic solution of stiff (and non-stiff) ODE. Gear et al.(1974) and Gear and Tu(1974) examine the effect of a changing mesh size on the stability of multi step methods. Skelboe(1977) studied control of order and step-size for multistep methods when one of the eigenvalues is close to the imaginary axis; an instability test is provided to automatically pick-up on when this is the case. Lindberg(1977) characterizes the optimal step-size sequence for stiff methods. See also the section in this review on start-up.

STIFFNESS DETECTION

The automatic detection of stiffness is related to the question of automatic method selection, that is, the choice of a stiff or non-stiff method. Gear(1980) recommends that initially a

non-stiff method always be used. Petzold(1980) and Petzold(1982) discusses a technique that uses information available at the end of each step to make a decision between continuing with a stiff or a non-stiff method. Shampine and Hiebert(1977) report a simple but effective method for following occurance of stiffness by use of the Runga-Kutta Fehlberg (4,5) formulas; also see Shampine(1977).

Kennealy and Moore(1977) show a heuristic method for detecting stiffness in mass-action kinetics. Braekhus and Aasen(1981) explore use of various explicit methods for detecting stiffness in problems of structural mechanics. See too Gladwell(1980).

Gordon and Shampine(1977) mention a code at Sandia, called DE, that solves non-stiff ODE but keeps a computer-eye out for the occurence of stiffness. These authors also identify two other very important ways of detecting stiffness, non-automatically: based on physical reasoning and based on computational experience with similar equations. There is another non-automatic way: through proper scaling of all variables, as would be done for a singular perturbation analysis or in preparation for putting the equations on an analog computer. See Flaherty and O'Malley(1979) for an automatic scheme for this scaling on a digitial computer.

Shampine(1980) reports a special definition of stiffness appropriate for implicit A-stable formulas; this definition can

be recognized using information already available during the integration. See also Sacks-Davis and Shampine(1981).

COMPARISON OF STIFF METHODS

Enright(1982) explains why it is not meaningful in general to compare different methods or packages containing different methods in order to arrive at a "best" method. However such comparisons can point to weaknesses in a method or code (Enright et al., 1975; Hull, 1980; Enright and Hull, 1976). As Enright mentions, it makes much more sense to compare different implementations of a given method, or to compare two related methods or packages. Byrne et al.(1977) compare GEAR and EPISODE with respect to appearance to the user, members of the package, features of software engineering, and the basic algorithms. EPISODE performs better than GEAR for problems involving waves or re-occuring stiffness, but GEAR is better for simple decaying problems.

Brown(1978) offers the program package STIFF-DETEST for comparison of stiff ODEs. See Weimar and Clough(1979) for a critical evaluation of the semi-implicit Runga-Kutta methods for stiff systems. Thompson(1977) and Bushard(1976) have performed comparisons. See also Scherer(1976), Carver et al.(1979), and Chan et al.(1978).

TEST PROBLEMS

Packaging considerations make it hard enough to compare methods, but the bottom line to evaluation of software is how well it works on "typical" stiff problems. Within selected application areas, there may be typical non-linear structure, degree of stiffness, and size, but in general there is not. One reasonable approach is to examine one application area only, or to examine many different test problems, representative of a spectrum of different applications.

Whichever approach is taken, there is virtue in consistency of choice. By far the most commonly used stiff ODE test problem is the three kinetics rate equation set of Robertson(1975, who cites the original 1966 article); we have counted at least 23 uses of this equation set in January,1974-March, 1982. Other favorites are given in Robertson(1975).

Enright et al.(1975) list five classes of stiff problems with a number of examples of each class: linear with real eigenvalues, linear with non-real eigenvalues, non-linear coupling(smooth to transient and transient to smooth), non-linear with real eigenvalues (most mass action kinetics problems are here), and non-linear with non-real eigenvalues; eigenvalue ranges are given for most of these. However Shampine(1977) and Shampine and Hiebert(1977) found several of the examples did not qualify , by their definition, as being stiff - although some

have other types of anomolous behavior. Shampine(1981) points out a number oF shortcomings with this test set and enumerates ways of improving it.

Enright and Hull(1976) give ten test problems involving chemical kinetics, in batch and more complex reactors. Johnson and Barney(1976) document eleven problems they used for testing. Hindmarsh and Byrne(1976) give a diurnal kinetics problem with the re-occuring stiffness feature characteristic of atmospheric reactions; they also have a simple diffusion-convection problem for use with the method of lines. A variety of test systems are offered by Michelsen(1976), including a large one and a differential- algebraic one. Chan et al.(1978) list eight stiff problems.

There are also available several testing equations of a rather special nature. Skelboe(1977) suggests stiff problems of a highly oscillatory nature, as does Gaffney(1982). Fatunla(1980) lists six examples, some of which are stiff and highly oscillatory. Dahlquist et al.(1980) give a simple stiff equation with a turning point, a stiff nonlinear oscillator, and a combustion example. Kreiss and Kreiss(1981) consider an example of a stiff two-point boundary value problem. Carver(1980) has two simple hyperbolic equations for testing: Burger's equation and a model for a counter-current heat exchanger.

ALGEBRAIC EQUATIONS

There has been little comparative advancement during recent years in solving linear or nonlinear equations relevant to ODE solvers, except for large sparse systems. However see Hindmarsh et al.(1978) for algorithmic advancements for dense linear LU decomposition. Johnson and Barney(1976) test five conventional methods for solving linear algebraic equations (MINV, SOLVE, DECOMP-SOLVE, JACOBI, AND GAUSS-SEIDEL). Byrne(1976) and Byrne and Hindmarsh(1977) consider solution of linear block tridiagonal forms arising from PDE descretization. Sherman and Hindmarsh(1980) consider solving the linear equations from Newton iteration on a nonlinear sparse set by the YSMP, Yale Sparse Matrix Package. See also Hindmarsh(1977) and the section in this review on sparse systems.

Shampine(1979) says that the solution of the algebraic equations from implicit ODE formulas is special. He found that the residual was the appropriate measure for acceptance of an approximate solution; a way to do this and the advantages are detailed.

Hindmarsh(1977) considers the idea of rank-one updates for the inverse of the Newton iteration matrix in the context of solving stiff ODEs, but the results are disappointing. Enright(1978) gives us a more efficient method for matrix factorization after a change in step-size or order, particularly

good for large dense systems. See Shampine(1981) for a pertinent discussion on Jacobians and stiff methods.Also Eitelberg(1979).

ANALOG COMPUTATION

There are some advantages for use of an analog computer for time-critical computation, that is for some real-time needs or for stiff computation. There has not been a widely-accepted recent evaluation of this usefullness, however. Reasons why analogs are used comparatively infrequently include the basic equipment expense (about a thousand dollars an integrator) to buy an analog for a laboratory that typically already has a digital computer. The digitial is much more versatile. Also there does not yet exist "software" in the digital sense. Therefore one must "patch" an analog manually, although this could be based on a diagram written by someone else. Another huge inconvienence is the need to scale the problem so that all variables vary on the same normalized interval a normalized amount. For stiff ODEs this is rather equilvalent to requiring the user set-up his problem in dimensionlessized singular perturbation form. However once this is done, the ease of parameter variation and the continuous graphical availability of the solution on an oscilloscope makes for an excellent environment to throughly explore sensitivities of parameters and interactions of variables nonlinearly related.

Our laboratory owns a hybrid EAI PACER 1000/580 system and

an EAI2000 analog (connected serially to an Apple digial computer). We have on-going work in the evaluation of the analog for stiff computation, as occurs from mass-action kinetic models of certain combustion reactions. We have noted an upper limit on the degree of stiffness that the analog can handle (for example eigenvalue spreads greater than about 10X6 seem impossible to solve); however there is likely to be a relation between a variable not solvable on the analog and a one that is really not that important to the overall solution. But this is often evident once the equations have been properly scaled, before being patched.

For solutions of stiff equations on a hybrid computer, reference is given to Kogan et al.(1980), Karba et al.(1980), Neundorf(1981), and El-Zorkany(1981). Stiff problems on an analog alone: Bernard-Weil et al.(1978).Refer to Gear(1977) for comments on the use of the digital for real-time dynamics.

DIFFERENTIAL-ALGEBRAIC

These occur in models of power systems, control systems and from application of the steady-state approximation or perturbation methods. They present particular problems with determining initial conditions, error estimation and step - size selection (Gear et al.1981). If the algebraic equation resulted from setting a derivative to zero, singly algebraic equations can

sometimes be solved explicitly and back-substituted, for example in chemical kinetics of the mass action form. If this elimination cannot be effected, the differential-algebraic set can exhibit the same stiffness as the original fully-differential set. Some problems cannot even be solved with stiff methods, without extensive modifications in the error estimates and other strategies of the code ; and sometimes they apparently cannot be solved at all by stiff methods(Petzold, 1981). See too her package DASSL (Petzold, 1982).

Liniger(1979) gives us multistep and one-leg methods for implicit mixed differential-algebraic systems. Soderlind(1980) has written DASP3, a program for partitioned stiff ODEs and differential-algebraic sets. Chua and Dew(1982) attack these mixed systems that also include discontinuities. Gross(1976) presents a method that makes special use of the structure in the differential-algebraic set;the nonlinear system is split into a stiff part with a sparse Jacobian and a nonstiff part. Datta and Martens(1974) investigate automatic step size selection techniques for a method tailored for this combination of equation types. Refer also to the algorithm of Starner(1976).

DIFFERENTIAL-DIFFERENCE

Delay terms arise in lossless transmission line modelling, in ecomonic modelling, and in ecological modelling, to name only a few areas. Brayton(1974) develops conditions for numerical A-stabilty for these systems. Bickart(1981) offers a program package for differential-difference systems. Van der Staay(1982) explores composite intergration-interpolation methods. Bickart(1982) determines F-stable and F(alpha, beta)-stable integration-interpolation methods. Weiderholt(1976) studies the stabiltity of multi-step methods for this class of mixed equation forms. Carver(1977) studied the efficient handling of discontinuities and time delays in ordinary differential equations. See also Roth(1980), Watanabe and Roth(1982), and Moore(1974).

DISCONTINUITIES

Ellison(1981) classifies events that cause discontinuities as either a time event or a state event. Automatic detection of time events is straight-forward, detection of state events is not but is achievable on examples given; an integration method schemes-up with the detection device for a program. Halin(1976) points out short comings of popular stiff software on discontimuities; he applies a "quasi-analytic" integration technique. De Doncker(1978) presents an automatic integration

algoritm (in QUADPACK) that makes use of a nonlinear extrapolation technique to jump discontinuities. Hay et al.(1974) also have a means for detection of a break and readjustment of the step so that the break is at the step's end.

GLOBAL ERROR

Users often do not realize that their integration package uses their requested accuracy requirement to match against ar estimate of the local error, not the actual error in the solution (global error). Lindberg(1977) shows for stiff problems the advantage of keeping the global error at the maximun allowable level during long intervals. Dahlquist(1981) reports work in progress to extend Lindberg's ideas to automatically control step size on the basis of global error; application is made to a system in partitioned form.

Dew and West(1978) consider estimating and controlling global error in Gear's method. Stetter(1974) considers global error estimation for non-stiff problems; Stetter(1979) global estimation in Adams predictor-corrector codes.

DECOUPLING

In addition to the obvious merits of smaller size, stiffness may find a better home in a "decoupled" or semi-decoupled subsystem. The steady-state approximation is the best known way of reducing order, but the differential-algebraic set(see this review) may be just as stiff. O'Malley and Anderson(1979) discuss how to find the small parameters automatically to do a steady-state approximation (the mathematically sound variety obtained by setting a parameter to zero rather than a derivative to zero); this is related to automatic partitioning.

Hofer advocates decoupling stiff from non-stiff, in large systems with only a few stiff variables, and using explicit techniques on the non-stiff part and implicit methods on the stiff part. Enright and Kamel(1980) study selection of a low-order linear model using the dominant mode concept; this is related to lumping and modelling questions.

Nandakumar and Andres(1978) explore a new class of algorithms that first heuristicaly decompose large systems into groups of smaller subsystems that share similar integration scales; they then solve individual subsystems and combine iteratively. Refer also to the decompositon methods, for stiff equations, of Clasen et al.(1978), Mattheij(1982), Burka(1982), and the problem-oriented studies of Anderson(1980) for control systems and Humpage et al.(1974) for power systems.

HIGHLY OSCILLATORY ODE

Gaffney(1982) has completed a critical survey and testing of software (STRIDE, BLEND, STINT, and DIRK) for solving stiff highly oscillatory ordinary differential equations; none of these packages are given very high marks on the test problem. There are also such things as highly oscillatory equations that do not qualify as being stiff in the usual sense (no large negative real eigenvalues), although they can be "stubborn".

Petzold(1981) presents a numerical method for this (non-stiff) highly oscillatory problem as does Fatunla(1980).Gear and Gallivan(1981) address automatic detection of highly oscillatory behavior, period determination, and efficeint integration. See also Gallivan(1980) and Gear(1980).

PARTITIONING

The practitioner may very well know which components are highly stable, that is stiff, and which are not. This information can be used to make the numerical solution more efficient for a variety of techniques. Most importantly, such knowledge could be used to make a modeling simplification to remove the highly stable component from the model, or to make a mathematical simplification to the problem: the steady-state approximation.

This approximation has the terrific property of being better the stiffer the system; it can be suprisingly accurate for even

weakly stiff systems. It is tricky to apply correctly for some systems, however (Aiken, 1982). The mathematical basis is a low-order outer approximation in singular perturbation theory and this can be quite different from merely mechanically setting a derivative equal to zero. A few recent interesting applications of the ad hoc version of the approximation are: Chen et al.(1979), Devooght and Mund(1980), Kao(1980), Farrow and Graedel(1977), Aronowitz et al.(1977), Warner(1977), Cao and Joesph(1979), and sophisticated versions in O'Malley and Anderson(1979) and O'Malley and Flaherty(1980). Application to the initial conditions can eliminate the initial transient (Aiken and Lapidus, 1975; Alfeld, 1980).

Soderlind(1979) discusses some stability properties of linear multistep compound methods on a system partitioned into two sections. Different techniques are used on each section. Palusinski and Wait(1978) examine methods on stiff partitioned systems into one linear and one nonlinear system and into two nonlinear systems. Andrus(1979) also took this two section, two method route. See also Soderlind(1980), Soderlind(1981) and Dahlquist(1981). Enright and Kamel(1979), Carver(1982), and Dahlquist and Fu-Fan(1982) are working on automatic partitioning.

SPARSE SYSTEMS

Large systems (more than ,say ,100 equations) are often sparse because there are usally direct interactions among only a few variables in the set. This is true, for example, in large kinetic rate equations. Large systems resulting from descretization of PDEs are sparse with special structure. Special handling of the sparsity can both reduce storage and computation time. Curtis(1977) reviews the state of the art.

Because the efficency of Gear's method depends heavily on the efficiency of matrix operations, particularly for larger systems, Hindmarsh(1974) provided a more versatile package, called GEAR that provided several matrix options: the Chord method, the diagonal method, and functional iteration. Later, he added an option for banded matrices, as from PDEs, in GEARB(Hindmarsh, 1975). The banded structure also occurs in models of stage-wise processing (Tyreus et al., 1975). Carver and Baudouin(1976) used this package to solve a stiff set of 242 ODEs modelling neutron kinetics and transport; they found that only the chord method allowed the solution to be reached in reasonable time but storage was near to machine capacity and 20 seconds were required for each Jacobian evaluation and decomposition. They therefore added to the package a method from the Harwell subroutine library for solution of large linear equations, which stores only non-zero entries and uses a pivotal scheme optimal in

some sense. The resulting package is called FORSIM. The greatest savings was probably in the numerical approximation to the Jacaobian: the matrix is evaluated first to find non-zero elements; then the Jacobian is evaluated by perturbing as many of the individual variables as effect only one derivative.

Sherman and Hindmarsh(1980) present GEARS, a package for stiff sparse ODE, using YSMP (Yale Sparse Matrix Package). The two main sparse techniques here are a special method for computing finite difference approximations to the Jacobian and YSMP non-pivoting Gausian elimination linear equation solver.

Schaumberg et al.(1980) and Zlatev et al.(1980) analyze implementation of a Gustavson storage scheme and a generalized Markowitz pivotal strategy for large stiff linear ODEs. Enright(1979) also examines stiff sparse linear ODEs, and suggests modifications to GEAR for three classes of linear equtions and four levels of structure.Guy Rabbat et al.(1979) mention sparse matrix techniques have allowed time domain analysis of circuits with hundreds of elements, but large scale integrated circuits present the challenge of solving thousands of active devices. Johnson and Barney(1976) look at several sparse techniques (SIMULT, IMP, and LINEQ4).

For strategies solving applications resulting in PDEs-turned ODEs, see Iserles(1981), Sincovec and Madsen(1975), Melgaard and

Sincovec(1981), Hunding(1980) and Karasalo and Kurylo(1981). The many other example implementations of sparse techniques include: Franke(1980), transient field problems; Watson(1976) for CSMP III; Gross(1976) for power systems; Carver et al.(1979) for mass-action kinetics; Dove and Raynor(1979, 1982), molecular dynamics; Enright(1980), structural mechanics; Sincovec et al.(1981) for describer systems; Prasad and Huntress(1980), interstellar clouds; Atkinson et al.(1980) , atmospheric pollution; and Thompson and Tuttle(1982) for process problems.

UNSTABLE PROBLEMS

Lindberg(1974) discusses the fact that many stiff methods fail to detect inherent instabilty of an equation, particularly when large negative eigenvalues turn positive. Aiken(1982) notes automatic methods can skip over an explosion in the model. Aiken(1982) notes a very common and very "stubborn" numerical problem in studying selectivity in gas purification operations, related to the occurence of positive eigenvalues. Hoppensteadt et al.(1981) propose a numerical method that focuses on the positive eigenvalues. Brown(1978) examines the error behavior of multistep methods applied to unstable differential equations.

PACKAGES

Most recent stiff packages generally available are mentioned in various sections of this review. Table I presents a summary of most of these. Lawrence Livermore National Laboratory (LLNL) has led the way for developing general and special purpose stiff packages for the user. Outside of LLNL, GEAR can be obtained from the National Energy Software Center(NESC), Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439; identify GEAR as NESC No. 592.

TABLE I. STIFF SOFTWARE

NAME	COMMENT	REFERENCE
General		
DGRUNG	Two-stage semi-implicit Runge-Kutta	Boness(1979)
EPISODE	Re-occuring stiffness	Byrne(1981)
FACSIMILE		Curtis(1980)
GEAR	Derived from DIFSUB	Hindmarsh(1974)
GRK4T	Rosenbrock methods	Kaps and Rentrop(1979)
IMP	Implicit midpoint	Lindberg(1974)
LSODE	More ease,flexiblity	Hindmarsh(1980)
SDBASIC	Second-derivative	Enright(1975)
STIFF 3	Semi-implicit R-K	Michelsen(1976)
STINT	Cyclic	Tendler et al.(1978)
STRIDE	Implicit R-K	Butcher, et al.(1979)
TRAPEX	Extrapolation	Enright et al.(1975)
Direct Variants of GEAR		
DSTPGT		Thompson and Tuttle(1982)
GEARS	Sparsity	Hindmarsh(1979)
GEARBI	2-3 dimensional PDE	Hindmarsh(1979)
GEARV	For parallel processors	Morris et al.(1979)
Special Applications		
CAKE	Kinetics	Ridler(1977)
CSDT	PDE, adjust mesh	Janac(1978)
DISPL2	Collocation-B-splines	Byrne(1981)
FORSIM VI	Sparse techniques	Carver(1979)
KINRATE	Kinetics	Edsberg(1974)
KISS	Kinetics	Gottwald(1981)
LARKIN	Large kinetics	Bader et al.(1982)
SETKIN	Kinetics preprocessor	Dickinson and Gelinas(1976)
Diferential-Algebraic		
DASP3	Also partitioning	Soderlind(1980)
DASSL		Petzold(1982)
EPISODEIB	Banded Jacobian	Hindmarsh(1979)
FAST	Transulator	Stutzman et al.(1976)
GEARIB	Banded Jacobian	Hindmarsh(1979)
GEMS	Extension of IMP	Babcock et al.(1981)
LSODEI	Linearly implicit	Hindmarsh(1980)
Process Simulation		
CSMP		Hylton(1982)
CSMP III		Watson and Gourlay(1976)
DPS		Sebastian et al.(1981)
DYNSYL		Patterson and Rozsa(1978)

REFERENCES

References are listed at the end of Part III.

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STIFF REVIEW 1974-1982: III.THEORY(LISTING)

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Subject listing in alphabetical order (note various stability types are listed by heading under STABILITY.

AVERAGING

Miranker(1982); Hoppensteadt(1979); Miranker(1978); Persek and Hoppensteadt(1978); Hoppensteadt and Miranker(1977); Coleman et al.(1977); Liniger(1976).

BLENDED

Cash(1981, 1982); Skeel and Kong(1977).

BLOCK

Bond and Cash(1979).

COLLOCATION

Burka(1982); Finlayson(1982); Dias et al.(1982); Chin et al.(1979); Guertin et al.(1977); Varma et al.(1976); Wouk(1976); Bushard(1976); Shah and Paraskos(1975); Serth(1975); Carey and Finlayson(1975); Michelsen and Villadsen(1974); Karanth and Hughes(1974); Scholander and Svedberg(1974); Brunner(1974).

CONTRACTIVE

Liniger(1982); Soderlind(1981); Mingyou(1981); Ruehli et al.(1980); Odeh and Liniger(1980); Dahlquist and Jeltsch(1979); Nevanlinna and Liniger(1979); Dahlquist(1979); Nevanlinna and Liniger(1978).

COMPOSITE MULTI-STEP

Tendler et al.(1978); Lucey(1975); Bickart(1974).

CYCLIC

Gupta(1979); Tendler et al.(1978); Mihelcic(1978); Michelcic(1977); Cash(1977).

DEFECT CORRECTION

Ueberhuber(1979); Frank and Ueberhuber(1977).

DELAY

Bickart(1982); Cryer(1974).

DISCONTINUOUS

Chua and Dew(1982); Struwe(1981); Tuttle(1981); O'Malley and Flaherty(1980); Halin(1979); Srivastava et al.(1979); De Doncker(1978); Mannshart(1978); De Hoog and Weiss(1977); Carver(1977); Halin(1976); Luke et al.(1976); Luke et al.(1975); Macccomack and Paullay(1974); Hay et al.(1974).

EXPLICIT

Fatunla(1980); Alfeld(1979); Kubicek and Visnak(1974).

EXPONENTIAL FITTING

Cash(1981); Iserles(1981); Cash(1981); Raptis(1980); Rentrop(1980); DeGroen and Hamker(1979); Miller(1979); Iserles(1979); Strehel and Peper(1979); Miranker(1978);

Norsett(1978); Iserles(1978); Rosenbaum(1978); Iserles(1977); Murphy(1977); Gear(1977); Jackson(1976); Ehle(1975); Sarkany and Liniger(1974); Jackson and Kenue(1974); Chu and Berman(1974); Makela et al.(1977); Chun-Yat(1974); Meister(1974).

EXTRAPOLATION

Duff and Nowak(1982); Hoppensteadt and Miranker(1979); Lawrence and Dorning(1977); Gladwell(1976); Cash(1976); Lindberg(1974).

FUNCTIONAL FITING

Iserles(1977).

HYBRID METHODS

Fatunla(1982); Jain and Jain(1981).

IMPLICIT EULER

Frank and Ueberhuber(1977).

LINEAR MULTISTEP

Nolting(1982); Liniger(1981); Van Veldhuizen(1981); Butcher(1981); Fatunla(1980); Sinha(1980); Gear(1980); Warming and Beam(1979); Soederling(1979); Dahlquist(1979); Alfeld(1979); Grigorieff and Schroll(1978); Dahlquist(1978); Jeltsch(1978); Varah(1978); Nevanlinna(1977); DeHoog and Weiss(1977); Jeltsch(1977); Kong(1977); Prothero(1976); Liniger(1975); Gupta

and Wallace(1975); Williams and De Hoog(1974).

MULTIDERIVATIVE

Cash(1981); Burrage(1980); Jeltsch(1979); Jeltsch(1977); Brown(1977); Jeltsch(1976); Fuchs(1976); Gennin(1974).

NONLINEAR MULTISTEP

Lee and Preiser(1978); Lee(1974).

ONE STEP

Van Brokhoven(1980); Cash(1978); Mannshart(1978); Watanabe(1978); Cash(1975); Prothero and Robinson(1974); Van Veldhuizen(1974); Brunner(1974); Norsett(1974).

ONE LEG

Liniger(1982); Sand(1981); Dahlquist et al.(1980); Brown(1979); Nevanlinna and Liniger(1979); Dahlquist(1979); Liniger(1979); Dahlquist(1978).

ORDER STARS

Hairer(1979); Wanner et al.(1978).

OSCILLATORY EQUATIONS

Miranker(1982); Fatunla(1982); Jain and Jain(1981); Petzold(1981); Cash(1981); Gourlay(1980); Ruehhli et al.(1980); Brown(1980); Fatunla(1980); Rinzel and Miller(1980); Warming and

Beam(1979); Hoppensteadt(1979); Hoppensteadt and Miranker(1979); Bui(1979); Kreiss(1979); Auslander and Miranker(1979); Jain and Jain(1979); Ruehli et al.(1978); Miranker and Veldhuizen(1978); Miranker(1978); Jeltsch(1978); Hoppensteadt and Miranker(1977); Skelboe(1977); Smith(1977); Amdursky and Ziv(1977); Lambert and Watson(1976); Miranker and Wahba(1976); Fatunla(1976); Gupta(1976); Snider and Fleming(1974).

QUADRATURE

Iserles(1981).

RUNGE-KUTTA

Implicit

Cash(1982); Zlatev(1981); Hundsdorfer and Spijker(1981); Mingyou(1981); Cash(1981); Burrage(1979); Van der Houwen(1979); Bui and Bui(1979); Burrage and Butcher(1979); Crouzeix(1979); Scherer(1979); Dahlquist and Jetsch(1979); Eitelberg(1979); Curtis(1979); Butcher(1979); Varah(1979); Freidli(1978); Burrage(1978); Palusinski(1978); Iserles(1978); Alexander(1977); Bickart(1977); Butcher(1976); Fuchs(1976); Cash(1975); Ehle(1975); Ehle and Lawson(1975).

Semi-explicit

Cooper(1979).

Semi-implicit

Cash(1982); Prokopakis and Seider(1981); Weimer and Boness(1979); Kaps(1979); Clough(1979); Cash(1979); Bui(1979);

Kaps and Rentrop(1979); Burrage(1978); Lapidus et al.(1978); Freidli(1978); Cash(1976); Michelsen(1976).

SINGLY IMPLICIT

Burrage(1980).

SECOND DERIVATIVE

Sacks-Davis and Shampine(1981); Sacks-Davis(1980): Enright(1978); Gupta(1978); Sacks-Davis(1977); Kennealy and Moore(1977); Hill(1976); Brown(1976); Kubicek and Visnak(1974); Enright(1974).

SECOND ORDER EQUATIONS

Addison(1980); Odeh and Liniger(1980); Heinrich and Zienkiewicz(1979); Van der Houwen(1979); Hairer(1979); Gear(1978); Jensen(1976); Liniger and Gagnebin(1974).

SEPARABLY STIFF

Lambert(1981).

SINGULAR PERTURBATION

Mattheij(1982); Mattheij and O'Malley(1982); Kreiss and Kreiss(1981); Petzold(1981); Soerderlind and Dahlquist(1981); Smith(1981);Sanchez-Palencia and Lobo-Hidalgo(1980); DeVooght and Dahlquist et al.(1980); Mund(1980); Kahil and Kokotovic(1980); Barton(1980); O'Malley and Flaherty(1980); Brandt(1979); Auslander and Miranker(1979); De Groen and Hamker(1979); Heinrich

and Zienkiewicz(1973); Michell and Christie(1979); Hsiao and Jordan(1979); Mattheij(1979); Miller(1979); Flaherty and O'Malley(1979); Bourgeat and Tapiero(1979); Andrus(1979); Hoppenstesdt and Miranker(1979); Come(1979); Hoppensteadt(1979); Kreiss(1979); Miranker(1978); Emel'yanov(1978); Persek and Hoppensteadt(1978); David(1977); Flaherty and O'Malley(1977); Robertson(1975); Aiken and Lapidus(1975); Flaherty and O'Malley(1975); Dontchev(1974); Kreiss(1974); Aiken and Lapidus(1974).

SPLINES

Rentrop(1980); Hill(1976).

STABILITY

General

Butcher(1981); Lambert(1980); Brown(1979); Jury(1978); Dahlquist(1978); Glaser(1978); Bickart and Jury(1978); Jury(1977);Dahlquist(1976).

A-stable

Bui and Poon(1981); Zlatev(1981); Iserles(1981); Odeh and Liniger(1980); Tadeusiewicz(1980); Van Brokhoven(1980); Wanner(1980); Galantai(1980); Burrage and Butcher(1979); Bui(1979); Warming and Beam(1979); Cooper and Sayfy(1979); Scraton(1979); Kaps(1979); Tripathy and Rao(1978); Bickart and Jury(1978); Dahlquist(1978); Iserles(1978); Jeltsch(1978); Wanner

et al.(1978); Watanabe(1978); Lee and Preiser(1978); Triqiante(1977); Brown(1977); Butcher(1977); Jeltsch(1977); Lombardi(1977); Fuchs(1976); Liniger(1976); Chipman(1976); Wanner(1976); Jackson(1976); Jeltsch(1976); Cash(1976); Cash(1975); Ehle and Lawson(1975); Butcher(1975); Ehle(1975); Prothero and Robinson(1974); Williams and De Hoog(1974); Marzulli(1974); Brandon(1974); Brayton(1974); Liniger and Gagnebin(1974); Norsett(1974); Axelsson(1974); Genin(1974); Nevanlinna and Sipila(1974).

<u>A(alpha) Stable</u>

Galantai(1980); Kaps(1979); Bickart and Jury(1978); Grigorieff and Schroll(1978); Michelcic(1978); Jeltsch(1977); Liniger(1975).

<u>A(alpha,r) Stable</u>

Nolting(1982).

<u>A(0) Stable</u>

Rodabaugh and Thompson(1979); Freidli and Jeltsch(1978); Jeltsch(1976); Liniger(1975).

<u>A0 Stable</u>

Jeltsch(1976).

<u>An Stable</u>

Zlatev(1981).

<u>Algebraically Stable</u>

Burrage(1978).

<u>Almost A Stable</u>

Mihelcic(1977).

Asymptotically Stable

Krogh(1981).

B Stable

Hundsdorfer(1981); Burrage and Butcher(1979); Crouzeix(1979); Scherer(1979); Jeltsch(1979); Dahlquist and Jeltsch(1979).

D Stable

Veldhuizen(1981).

F Stable

Bickart(1982).

G Stable

Dahlquist(1978); Nevanlinna(1976).

I Stable

Wanner et al.(1978).

L Stable

Scraton(1981); Day(1980); Cash(1980); Lambert(1980); Bui(1979); Scraton(1979); Bui(1979); Eitelberg(1979); Fatunla(1978); Bui(1977); Trigiante(1977).

L(alpha) Stable

Cash(1980).

L(0) Stable

Gourlay(1980).

Ln Stable

Zlatev(1981).

Nonlinear Stability

Dahlquist(1982); Soederlind(1981); Burrage and Butcher(1980); Burrage(1980); Brown(1979); Burrage and Butcher(1979); Dahlquist(1978); Burrage(1978); Cooper and Whiworth(1978); Rodabaugh and Thompson(1978); Trigiante(1977);

Liniger(1977); Nevanlinna(1977); Wanner(1976); Liniger and Odeh(1976); Dalquist(1975); Butcher(1975); Lambert(1974); Brandon(1974).

P Stable

Bickart(1982); Fatunla(1982); Jain and Jain(1981); Cash(1981); Jain and Jain(1979).

S Stable

Day(1980); Alexander(1977); Verwer(1977); Prothero and Robinson(1974).

Stiffly A Stable

Ehle and Lawson(1975).

Stiffly Stable

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Strong A Stable

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Strongly Stable

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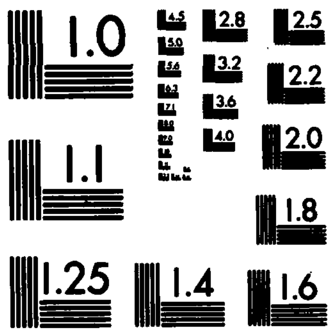

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